

10/575627

\*\*\*\*\* QUERY RESULTS \*\*\*\*\*

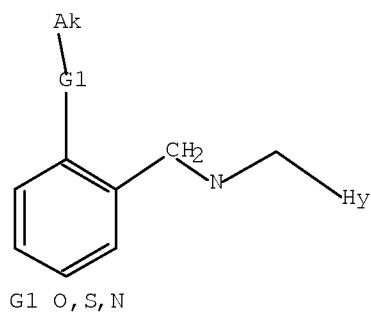
=> d his l15

(FILE 'REGISTRY' ENTERED AT 08:13:58 ON 06 MAR 2009)  
SAVE TEMP L14 DAV627REGL12/A

FILE 'HCAPLUS' ENTERED AT 08:20:42 ON 06 MAR 2009  
L15 0 S L14

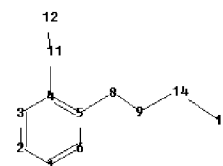
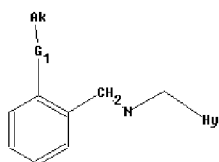
=> d que l15

L1 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L2.str



chain nodes :  
8 9 11 12 14 15  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
4-11 5-8 8-9 9-14 11-12 14-15  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
4-11 9-14 11-12 14-15  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6

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isolated ring systems :  
containing 1 :

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS  
12:CLASS

14:CLASS 15:Atom

Generic attributes :

15:

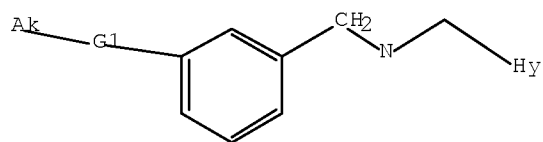
Saturation : Unsaturated

Element Count :

Node 12: Limited

C,C1-8

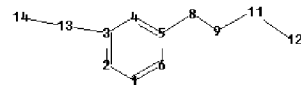
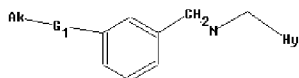
L2 ( 15347)SEA FILE=REGISTRY SSS FUL L1  
L3 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str



chain nodes :

8 9 11 12 13 14

ring nodes :

1 2 3 4 5 6

chain bonds :

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3-13 5-8 8-9 9-11 11-12 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
3-13 9-11 11-12 13-14  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O,S,N

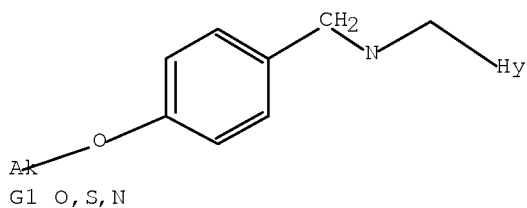
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS  
Generic attributes :  
12:  
Saturation : Unsaturated

Element Count :

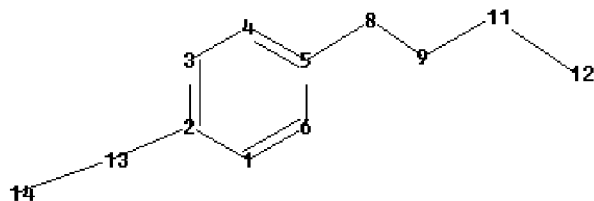
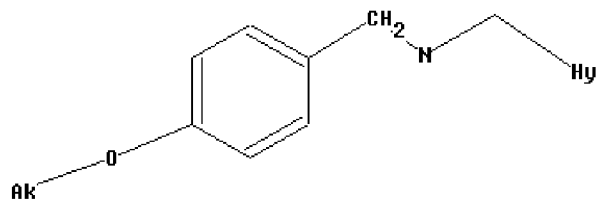
Node 14: Limited  
C,C1-8

L4 ( 22405)SEA FILE=REGISTRY SSS FUL L3  
L5 SCR 2043 OR 1918  
L6 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L5.str



chain nodes :

8 9 11 12 13 14

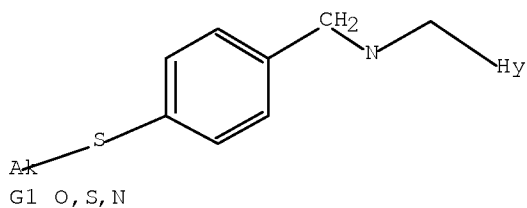
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ring nodes :  
1 2 3 4 5 6  
chain bonds :  
2-13 5-8 8-9 9-11 11-12 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
2-13 9-11 11-12 13-14  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O,S,N

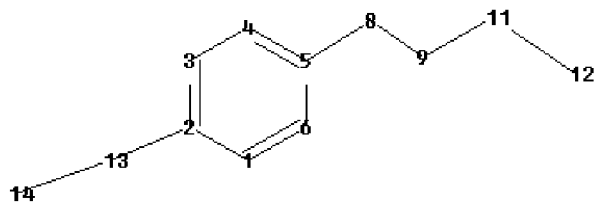
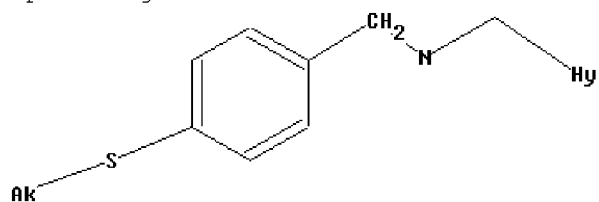
Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS  
Generic attributes :  
12:  
Saturation : Unsaturated  
  
Element Count :  
Node 14: Limited  
C,C1-8

L7 ( 26302)SEA FILE=REGISTRY SSS FUL L6 NOT L5  
L8 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L6.str



chain nodes :  
 8 9 11 12 13 14  
 ring nodes :  
 1 2 3 4 5 6  
 chain bonds :  
 2-13 5-8 8-9 9-11 11-12 13-14  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6  
 exact/norm bonds :  
 2-13 9-11 11-12 13-14  
 exact bonds :  
 5-8 8-9  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6  
 isolated ring systems :  
 containing 1 :

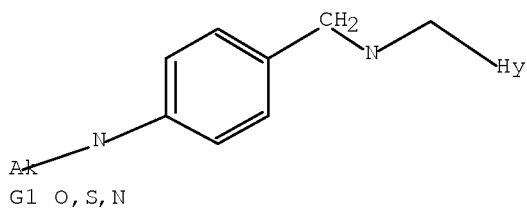
G1:O,S,N

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
 13:CLASS 14:CLASS  
 Generic attributes :  
 12:  
 Saturation : Unsaturated

Element Count :  
 Node 14: Limited  
 C,C1-8

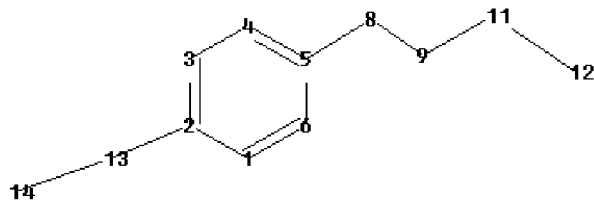
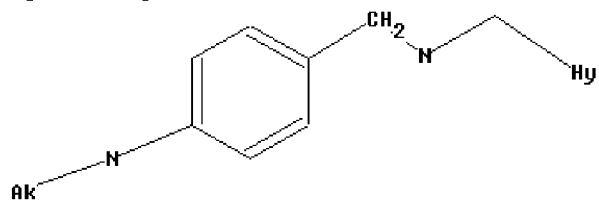
L9

STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L7.str



```

chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

```

G1:O,S,N

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes :
12:
Saturation          : Unsaturated

```

```

Element Count :
Node 14: Limited
C,C1-8

```

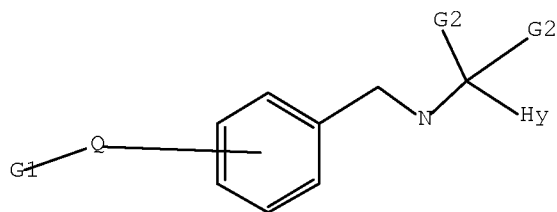
```

L10 (      5008)SEA FILE=REGISTRY SSS FUL L8 OR L9
L11      55683 SEA FILE=REGISTRY ABB=ON  PLU=ON  L2 OR L4 OR L7 OR L10
L12              STR

```

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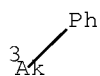
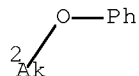
Ak<sup>4</sup>



Ak<sup>1</sup>

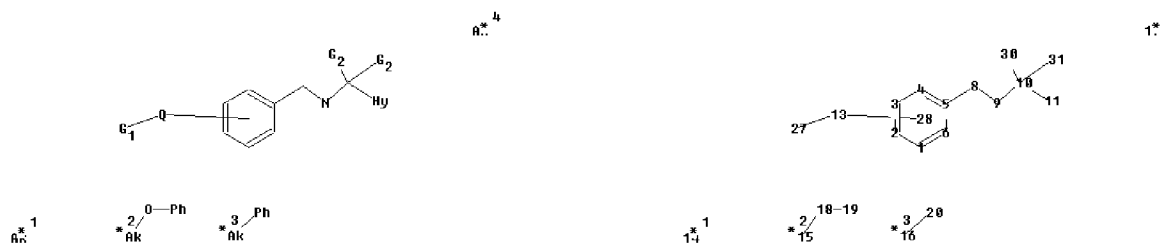
G1 [01], [02], [03]

G2 H, [04]



Structure attributes must be viewed using STN Express query preparation:

Uploading L12.str



chain nodes :

8 9 10 11 13 14 15 16 17 18 19 20 27 30 31

ring nodes :

1 2 3 4 5 6

chain bonds :

5-8 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 18-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20

exact bonds :

5-8 18-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

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G1:[\*1],[\*2],[\*3]

G2:H,[\*4]

Connectivity :

14:1 E exact RC ring/chain 17:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom  
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
27:CLASS 28:Atom  
30:CLASS 31:CLASS

Generic attributes :

11:

Saturation : Unsaturated

Element Count :

Node 11: Limited

C,C5-10

S,S1

Node 14: Limited

C,C3-8

Node 17: Limited

C,C1-3

L14 12 SEA FILE=REGISTRY SUB=L11 SSS FUL L12

L15 0 SEA FILE=HCAPLUS ABB=ON PLU=ON L14

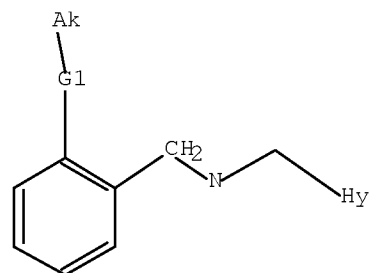
=> d his l14

(FILE 'REGISTRY' ENTERED AT 08:13:58 ON 06 MAR 2009)

L14 12 S L12 FUL SUB=L11

=> d que l14

L1 STR

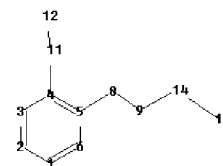
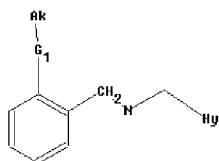


G1 O, S, N

Structure attributes must be viewed using STN Express query preparation:



Uploading L2.str



```
chain nodes :
8 9 11 12 14 15
ring nodes :
1 2 3 4 5 6
chain bonds :
4-11 5-8 8-9 9-14 11-12 14-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-11 9-14 11-12 14-15
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
```

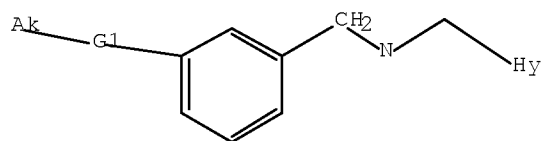
G1:O,S,N

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS
12:CLASS
14:CLASS 15:Atom
Generic attributes :
15:
Saturation : Unsaturated
```

```
Element Count :
Node 12: Limited
C,C1-8
```

```
L2 ( 15347)SEA FILE=REGISTRY SSS FUL L1
L3 STR
```

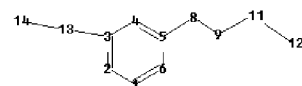
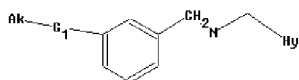
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G1 O, S, N

Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str



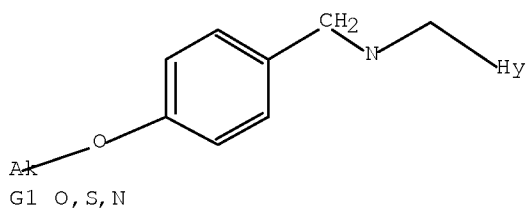
chain nodes :  
8 9 11 12 13 14  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
3-13 5-8 8-9 9-11 11-12 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
3-13 9-11 11-12 13-14  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O, S, N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS  
Generic attributes :  
12:  
Saturation : Unsaturated

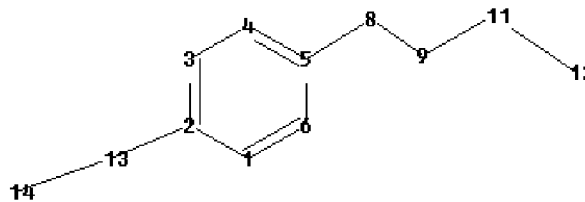
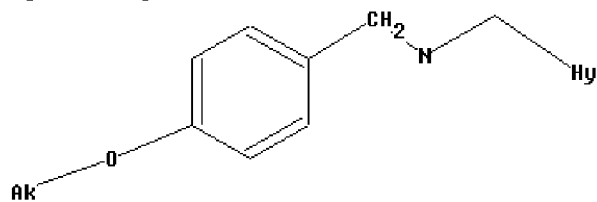
Element Count :  
Node 14: Limited  
C, C1-8

L4 ( 22405)SEA FILE=REGISTRY SSS FUL L3  
 L5 SCR 2043 OR 1918  
 L6 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L5.str



chain nodes :  
 8 9 11 12 13 14  
 ring nodes :  
 1 2 3 4 5 6  
 chain bonds :  
 2-13 5-8 8-9 9-11 11-12 13-14  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6  
 exact/norm bonds :  
 2-13 9-11 11-12 13-14  
 exact bonds :  
 5-8 8-9  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6  
 isolated ring systems :  
 containing 1 :

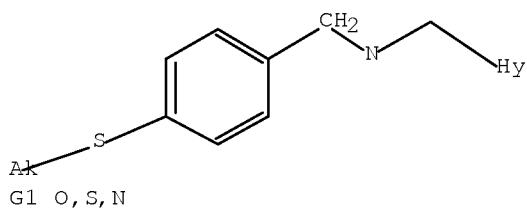
G1:O,S,N

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
 13:CLASS 14:CLASS  
 Generic attributes :  
 12:  
 Saturation : Unsaturated

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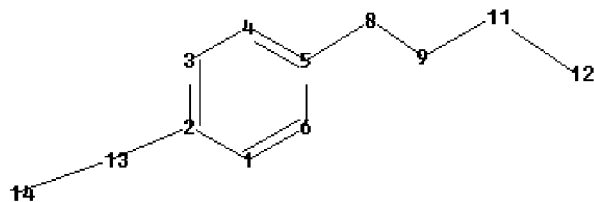
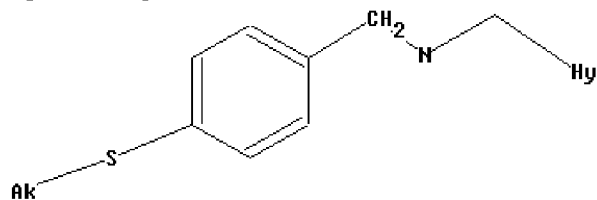
Element Count :  
Node 14: Limited  
C,C1-8

L7 ( 26302)SEA FILE=REGISTRY SSS FUL L6 NOT L5  
L8 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L6.str



chain nodes :  
8 9 11 12 13 14  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
2-13 5-8 8-9 9-11 11-12 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
2-13 9-11 11-12 13-14  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O, S, N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS  
Generic attributes :  
12:

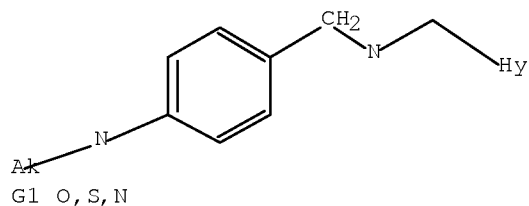
10/575627

Saturation : Unsaturated

Element Count :  
Node 14: Limited  
C,C1-8

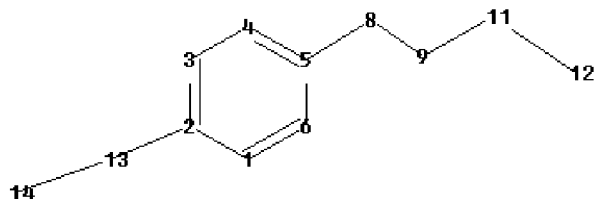
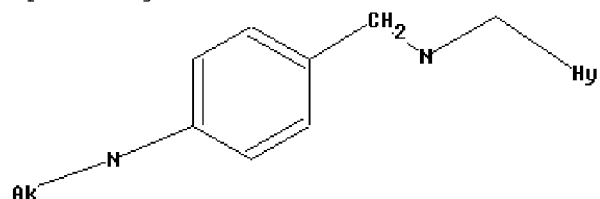
L9

STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L7.str



chain nodes :  
8 9 11 12 13 14  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
2-13 5-8 8-9 9-11 11-12 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
2-13 9-11 11-12 13-14  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O, S, N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS

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Generic attributes :

12:

Saturation : Unsaturated

Element Count :

Node 14: Limited

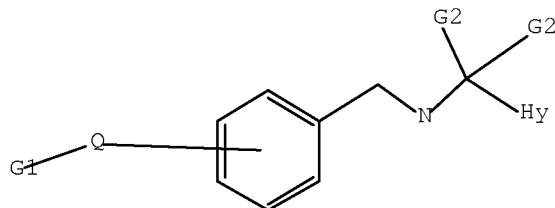
C,C1-8

L10 ( 5008)SEA FILE=REGISTRY SSS FUL L8 OR L9

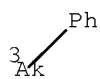
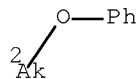
L11 55683 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR L4 OR L7 OR L10

L12 STR

Ak<sup>4</sup>



Ak<sup>1</sup>

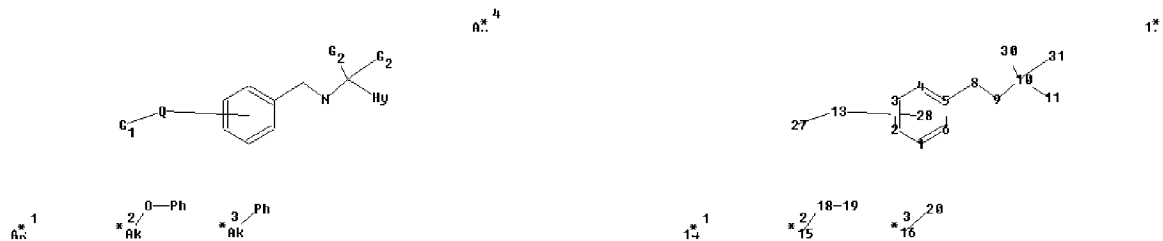


G1 [01], [02], [03]

G2 H, [04]

Structure attributes must be viewed using STN Express query preparation:

Uploading L12.str



chain nodes :

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8 9 10 11 13 14 15 16 17 18 19 20 27 30 31  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
5-8 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 18-19  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20  
exact bonds :  
5-8 18-19  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:[\*1],[\*2],[\*3]

G2:H,[\*4]

Connectivity :  
14:1 E exact RC ring/chain 17:1 E exact RC ring/chain  
Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom  
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
27:CLASS 28:Atom  
30:CLASS 31:CLASS  
Generic attributes :  
11:  
Saturation : Unsaturated

Element Count :  
Node 11: Limited  
C,C5-10  
S,S1

Node 14: Limited  
C,C3-8

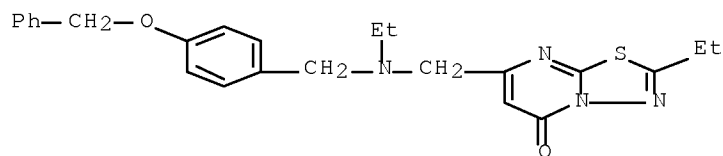
Node 17: Limited  
C,C1-3

L14 12 SEA FILE=REGISTRY SUB=L11 SSS FUL L12

=> d l14 1-12 ide

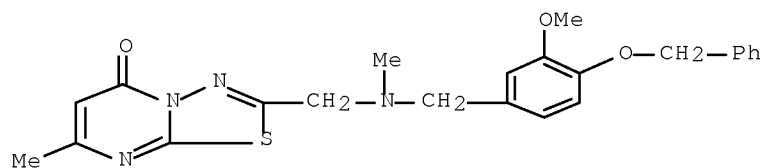
L14 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
RN 1090692-25-3 REGISTRY  
ED Entered STN: 28 Dec 2008  
CN INDEX NAME NOT YET ASSIGNED  
MF C24 H26 N4 O2 S  
SR Chemical Library  
Supplier: Ambinter

LC STN Files: CHEMCATS



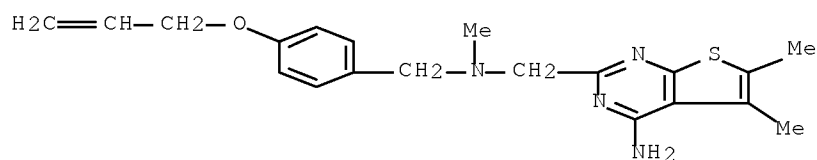
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 1089649-59-1 REGISTRY  
 ED Entered STN: 24 Dec 2008  
 CN INDEX NAME NOT YET ASSIGNED  
 MF C23 H24 N4 O3 S  
 SR Chemical Library  
 Supplier: Ambinter  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

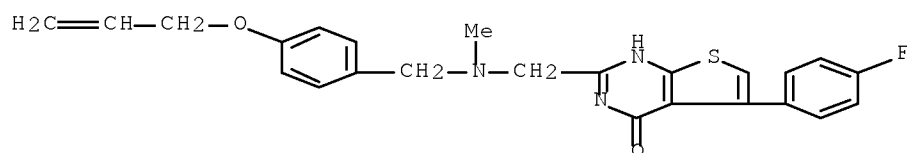
L14 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 1030752-95-4 REGISTRY  
 ED Entered STN: 26 Jun 2008  
 CN Thieno[2,3-d]pyrimidine-2-methanamine,  
 4-amino-N,5,6-trimethyl-N-[[4-(2-propen-1-yloxy)phenyl]methyl]- (CA INDEX  
 NAME)  
 MF C20 H24 N4 O S  
 SR Chemical Library  
 Supplier: Aurora Fine Chemicals  
 LC STN Files: CHEMCATS





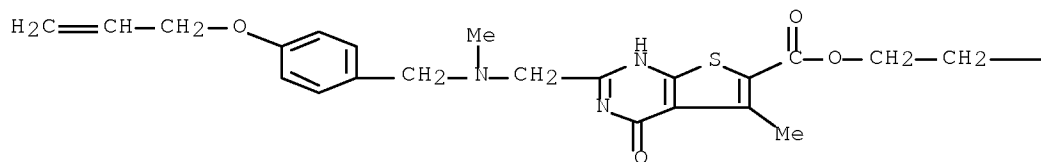
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 1013727-14-4 REGISTRY  
 ED Entered STN: 11 Apr 2008  
 CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5-(4-fluorophenyl)-2-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]- (CA INDEX NAME)  
 MF C24 H22 F N3 O2 S  
 SR Chemical Library  
 Supplier: Ambinter  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 1013599-48-8 REGISTRY  
 ED Entered STN: 10 Apr 2008  
 CN Thieno[2,3-d]pyrimidine-6-carboxylic acid, 1,4-dihydro-5-methyl-2-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]-4-oxo-, 2-methoxyethyl ester (CA INDEX NAME)  
 MF C23 H27 N3 O5 S  
 SR Chemical Library  
 Supplier: Ambinter  
 LC STN Files: CHEMCATS



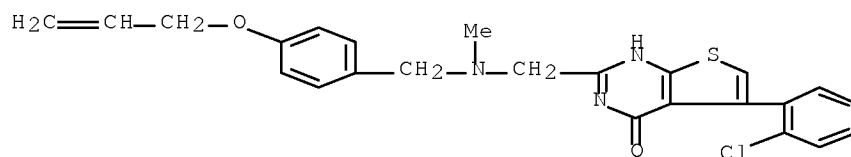
PAGE 1-A

PAGE 1-B

—OMe

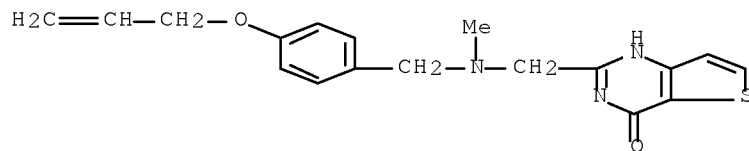
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 1013300-64-5 REGISTRY  
 ED Entered STN: 10 Apr 2008  
 CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5-(2-chlorophenyl)-2-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]- (CA INDEX NAME)  
 MF C24 H22 Cl N3 O2 S  
 SR Chemical Library  
 Supplier: Ambinter  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 949406-17-1 REGISTRY  
 ED Entered STN: 05 Oct 2007  
 CN Thieno[3,2-d]pyrimidin-4(3H)-one, 2-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]- (CA INDEX NAME)  
 MF C18 H19 N3 O2 S  
 SR Chemical Library  
 Supplier: Enamine  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 930905-89-8 REGISTRY  
 ED Entered STN: 19 Apr 2007  
 CN Thieno[2,3-d]pyrimidine-6-carboxylic acid,

10/575627

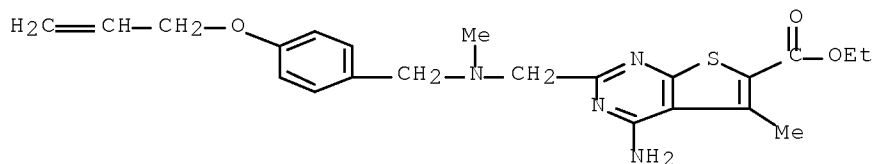
4-amino-5-methyl-2-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]-, ethyl ester (CA INDEX NAME)

MF C22 H26 N4 O3 S

SR Chemical Library

Supplier: Enamine

LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 930016-76-5 REGISTRY

ED Entered STN: 13 Apr 2007

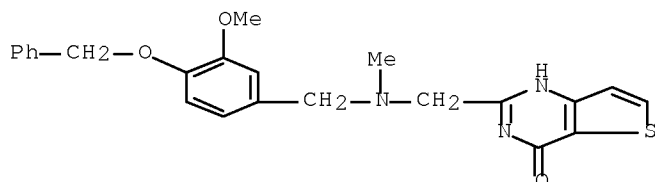
CN Thieno[3,2-d]pyrimidin-4(3H)-one, 2-[[[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]methylamino]methyl]- (CA INDEX NAME)

MF C23 H23 N3 O3 S

SR Chemical Library

Supplier: Enamine

LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 924238-94-8 REGISTRY

ED Entered STN: 02 Mar 2007

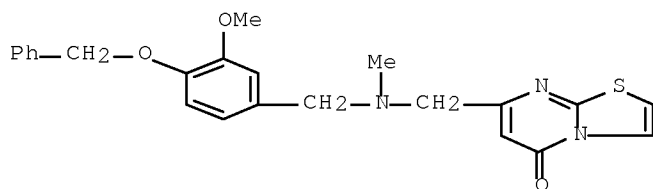
CN 5H-Thiazolo[3,2-a]pyrimidin-5-one, 7-[[[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]methylamino]methyl]- (CA INDEX NAME)

MF C23 H23 N3 O3 S

SR Chemical Library

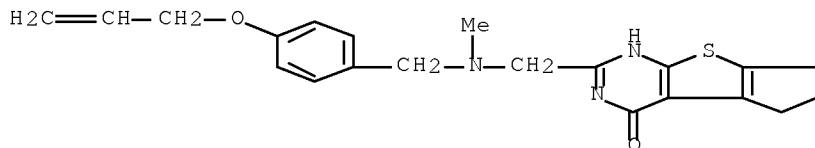
Supplier: Aurora Fine Chemicals

LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

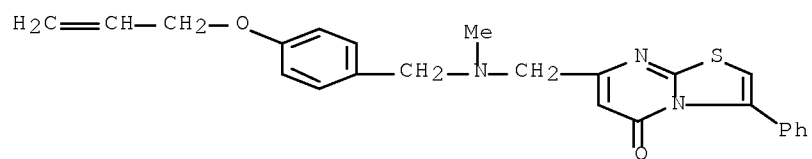
L14 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 876579-73-6 REGISTRY  
 ED Entered STN: 13 Mar 2006  
 CN 4H-Cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one,  
 1,5,6,7-tetrahydro-2-[[methyl[[4-(2-propen-1-  
 yloxy)phenyl]methyl]amino]methyl]- (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 4H-Cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one,  
 1,5,6,7-tetrahydro-2-[[methyl[[4-(2-  
 propenyloxy)phenyl]methyl]amino]methyl]- (9CI)  
 MF C21 H23 N3 O2 S  
 SR Chemical Library  
 Supplier: Aurora Fine Chemicals  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN  
 RN 871092-29-4 REGISTRY  
 ED Entered STN: 04 Jan 2006  
 CN 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
 7-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]-3-phenyl- (CA  
 INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
 7-[[methyl[[4-(2-propenyloxy)phenyl]methyl]amino]methyl]-3-phenyl- (9CI)  
 MF C24 H23 N3 O2 S  
 SR Chemical Library  
 Supplier: Enamine  
 LC STN Files: CHEMCATS

10/575627



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

=> d his l16

(FILE 'REGISTRY' ENTERED AT 08:21:32 ON 06 MAR 2009)

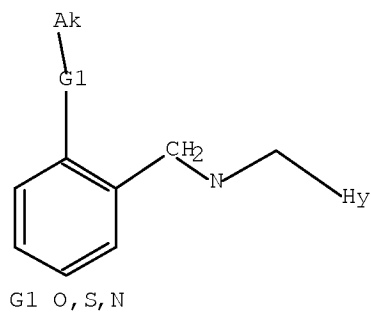
FILE 'CHEMCATS' ENTERED AT 08:58:39 ON 06 MAR 2009  
L16 30 S L14

FILE 'REGISTRY' ENTERED AT 09:01:42 ON 06 MAR 2009

FILE 'CHEMCATS' ENTERED AT 09:01:45 ON 06 MAR 2009

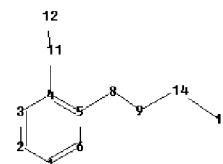
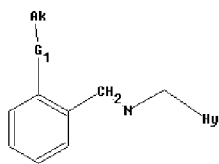
=> d que l16

L1 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L2.str



chain nodes :

8 9 11 12 14 15

ring nodes :

1 2 3 4 5 6

chain bonds :

4-11 5-8 8-9 9-14 11-12 14-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

10/575627

4-11 9-14 11-12 14-15  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS

12:CLASS

14:CLASS 15:Atom

Generic attributes :

15:

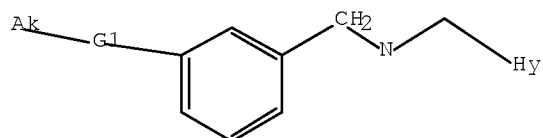
Saturation : Unsaturated

Element Count :

Node 12: Limited

C,C1-8

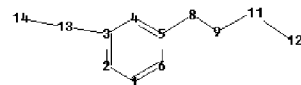
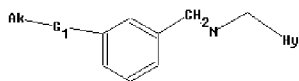
L2 ( 15347)SEA FILE=REGISTRY SSS FUL L1  
L3 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str



chain nodes :

10/575627

8 9 11 12 13 14  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
3-13 5-8 8-9 9-11 11-12 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
3-13 9-11 11-12 13-14  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS

Generic attributes :

12:

Saturation : Unsaturated

Element Count :

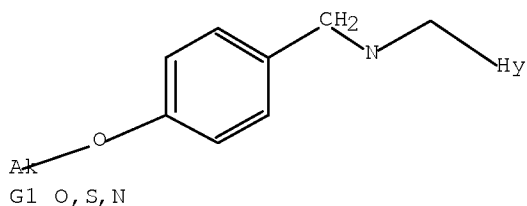
Node 14: Limited

C,C1-8

L4 ( 22405)SEA FILE=REGISTRY SSS FUL L3

L5 SCR 2043 OR 1918

L6 STR

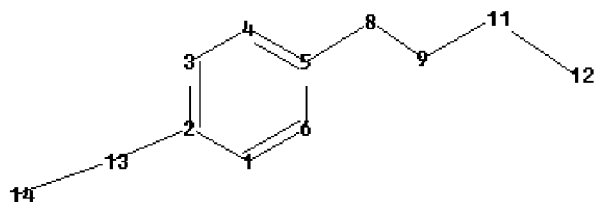
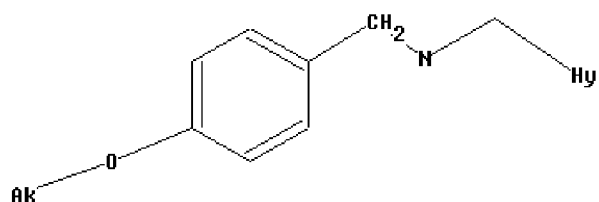


Structure attributes must be viewed using STN Express query preparation:

Uploading L5.str



10/575627



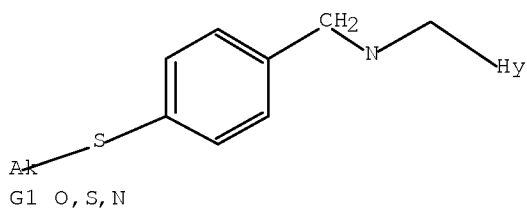
chain nodes :  
 8 9 11 12 13 14  
 ring nodes :  
 1 2 3 4 5 6  
 chain bonds :  
 2-13 5-8 8-9 9-11 11-12 13-14  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6  
 exact/norm bonds :  
 2-13 9-11 11-12 13-14  
 exact bonds :  
 5-8 8-9  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6  
 isolated ring systems :  
 containing 1 :

G1:O,S,N

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
 13:CLASS 14:CLASS  
 Generic attributes :  
 12:  
 Saturation : Unsaturated

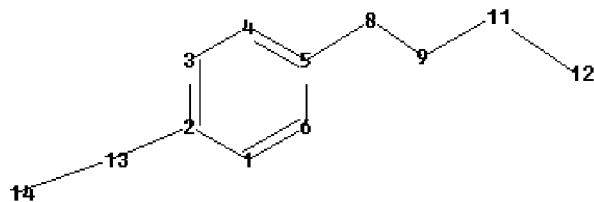
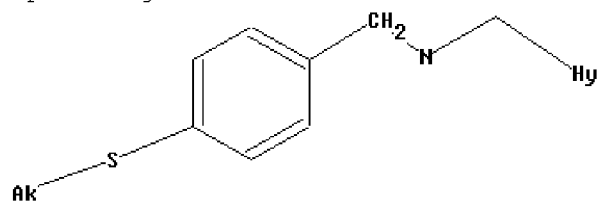
Element Count :  
 Node 14: Limited  
 C,C1-8

L7 ( 26302)SEA FILE=REGISTRY SSS FUL L6 NOT L5  
 L8 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L6.str



```

chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

```

G1:O,S,N

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS

```

Generic attributes :

12:

Saturation : Unsaturated

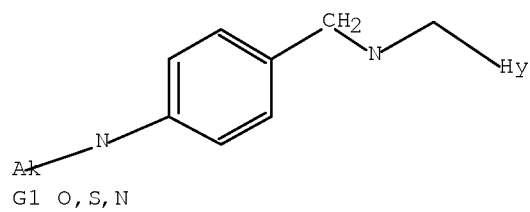
Element Count :

Node 14: Limited

C,C1-8

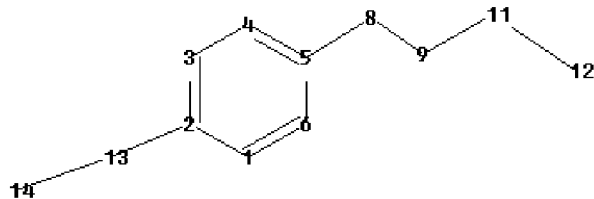
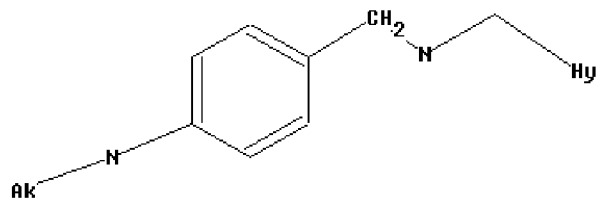
L9

STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L7.str



```
chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
```

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS

Generic attributes :

12:

Saturation : Unsaturated

Element Count :

Node 14: Limited

C,C1-8

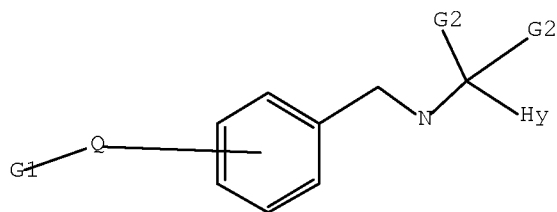
L10 ( 5008)SEA FILE=REGISTRY SSS FUL L8 OR L9

L11 55683 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR L4 OR L7 OR L10

L12 STR

10/575627

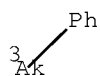
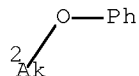
Ak<sup>4</sup>



Ak<sup>1</sup>

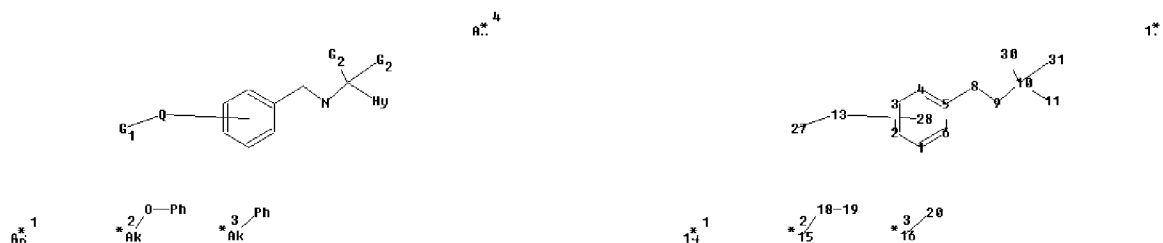
G1 [01], [02], [03]

G2 H, [04]



Structure attributes must be viewed using STN Express query preparation:

Uploading L12.str



chain nodes :

8 9 10 11 13 14 15 16 17 18 19 20 27 30 31

ring nodes :

1 2 3 4 5 6

chain bonds :

5-8 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 18-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20

exact bonds :

5-8 18-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[\*1],[\*2],[\*3]

G2:H,[\*4]

Connectivity :

14:1 E exact RC ring/chain 17:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom  
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
27:CLASS 28:Atom  
30:CLASS 31:CLASS

Generic attributes :

11:

Saturation : Unsaturated

Element Count :

Node 11: Limited

C,C5-10

S,S1

Node 14: Limited

C,C3-8

Node 17: Limited

C,C1-3

L14 12 SEA FILE=REGISTRY SUB=L11 SSS FUL L12

L16 30 SEA FILE=CHEMCATS ABB=ON PLU=ON L14

=> fil stng

FILE 'STNGUIDE' ENTERED AT 09:02:05 ON 06 MAR 2009

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Feb 27, 2009 (20090227/UP).

=> d l16 1-30 ide

L16 ANSWER 1 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2061673348 CHEMCATS

Catalog Name (CO): Ambinter Stock Screening Collection

Publication Date (PD): 21 Nov 2008

Order Number (ON): T6055864

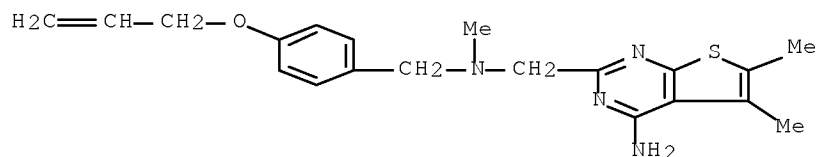
Chemical Name (CN): Thieno[2,3-d]pyrimidine-2-methanamine,  
4-amino-N,5,6-trimethyl-N-[[4-(2-propen-1-  
yloxy)phenyl]methyl]-

CAS Registry No. (RN): 1030752-95-4

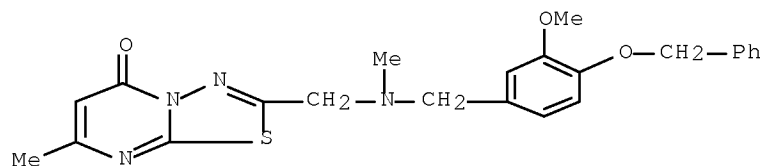
Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

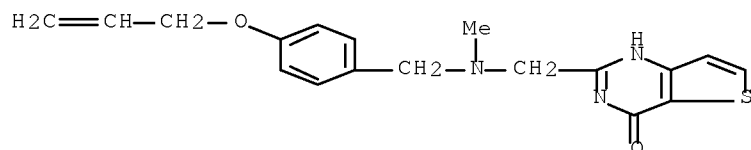
10/575627



L16 ANSWER 2 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
 Accession No. (AN): 2061042000 CHEMCATS  
 Catalog Name (CO): Ambinter Stock Screening Collection  
 Publication Date (PD): 21 Nov 2008  
 Order Number (ON): T6216377  
 Chemical Name (CN): Chemical name not yet assigned  
 CAS Registry No. (RN): 1089649-59-1  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



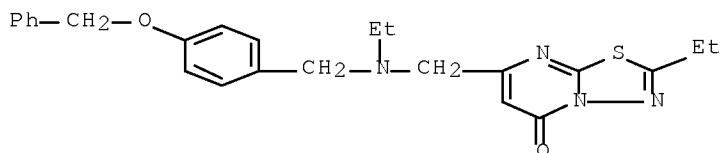
L16 ANSWER 3 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
 Accession No. (AN): 2060875760 CHEMCATS  
 Catalog Name (CO): Ambinter Stock Screening Collection  
 Publication Date (PD): 21 Nov 2008  
 Order Number (ON): T5954092  
 Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,  
 2-[[methyl[[4-(2-propen-1-  
 yloxy)phenyl]methyl]amino]methyl]-  
 CAS Registry No. (RN): 949406-17-1  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



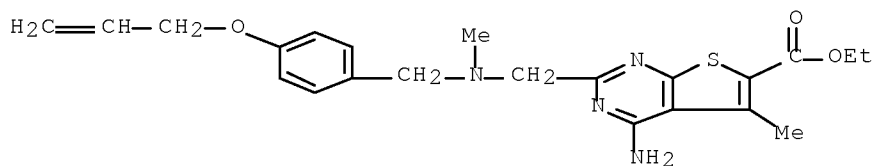
L16 ANSWER 4 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
 Accession No. (AN): 2060671762 CHEMCATS

10/575627

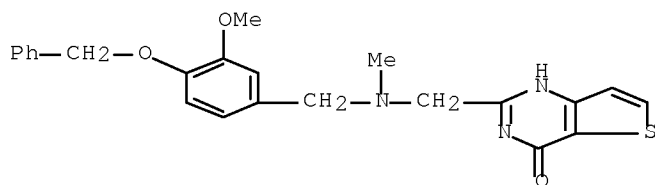
Catalog Name (CO): Ambinter Stock Screening Collection  
Publication Date (PD): 21 Nov 2008  
Order Number (ON): T6261100  
Chemical Name (CN): Chemical name not yet assigned  
CAS Registry No. (RN): 1090692-25-3  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



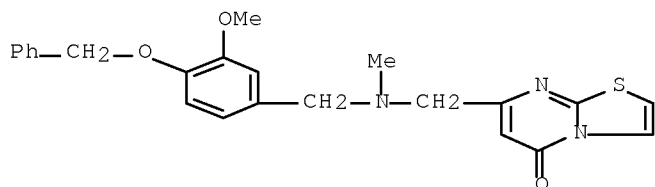
L16 ANSWER 5 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
Accession No. (AN): 2060237217 CHEMCATS  
Catalog Name (CO): Ambinter Stock Screening Collection  
Publication Date (PD): 21 Nov 2008  
Order Number (ON): T5833544  
Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,  
4-amino-5-methyl-2-[[methyl[[4-(2-propen-1-  
yloxy)phenyl]methyl]amino]methyl]-, ethyl ester  
CAS Registry No. (RN): 930905-89-8  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



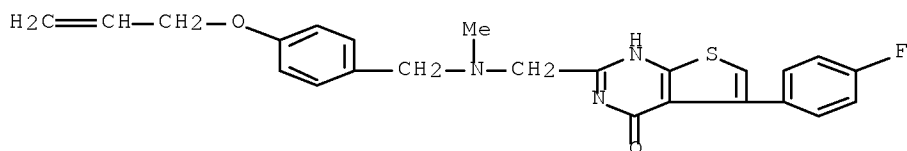
L16 ANSWER 6 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
Accession No. (AN): 2060226305 CHEMCATS  
Catalog Name (CO): Ambinter Stock Screening Collection  
Publication Date (PD): 21 Nov 2008  
Order Number (ON): T5810150  
Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,  
2-[[[[3-methoxy-4-  
(phenylmethoxy)phenyl]methyl]methylamino]methyl]-  
CAS Registry No. (RN): 930016-76-5  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



L16 ANSWER 7 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
 Accession No. (AN): 2060163673 CHEMCATS  
 Catalog Name (CO): Ambinter Stock Screening Collection  
 Publication Date (PD): 21 Nov 2008  
 Order Number (ON): T5682113  
 Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
 7-[[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]methylamino]methyl]-  
 CAS Registry No. (RN): 924233-94-8  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



L16 ANSWER 8 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
 Accession No. (AN): 2056291684 CHEMCATS  
 Catalog Name (CO): AKos Screening Library  
 Publication Date (PD): 18 Jul 2008  
 Order Number (ON): AKE-PB65201304  
 Chemical Name (CN): Thieno[2,3-d]pyrimidin-4(1H)-one,  
 5-(4-fluorophenyl)-2-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]-  
 CAS Registry No. (RN): 1013727-14-4  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

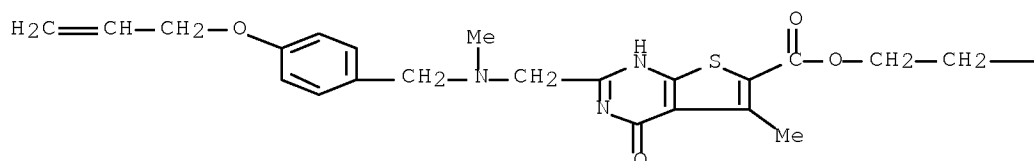




L16 ANSWER 9 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2055673608 CHEMCATS  
 Catalog Name (CO): AKos Screening Library  
 Publication Date (PD): 18 Jul 2008  
 Order Number (ON): AKE-PB-12658864  
 Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,  
 1,4-dihydro-5-methyl-2-[[methyl[[4-(2-propen-1-  
 yloxy)phenyl]methyl]amino]methyl]-4-oxo-,  
 2-methoxyethyl ester  
 CAS Registry No. (RN): 1013599-48-8  
 Supplementary Term (ST): CHEMICAL LIBRARY; CHEMICAL LIBRARY  
 Structure :

PAGE 1-A

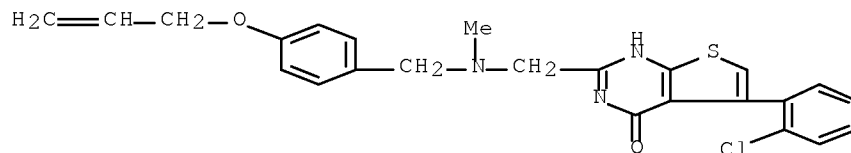


PAGE 1-B

—OMe

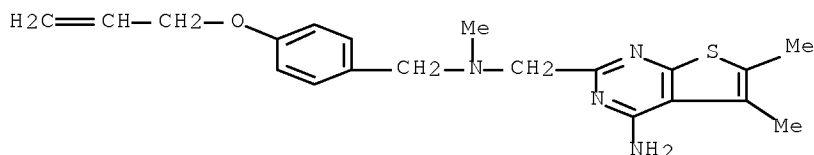
L16 ANSWER 10 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2055659677 CHEMCATS  
 Catalog Name (CO): AKos Screening Library  
 Publication Date (PD): 18 Jul 2008  
 Order Number (ON): AKE-PB-12658896  
 Chemical Name (CN): Thieno[2,3-d]pyrimidin-4(1H)-one,  
 5-(2-chlorophenyl)-2-[[methyl[[4-(2-propen-1-  
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 CAS Registry No. (RN): 1013300-64-5  
 Supplementary Term (ST): CHEMICAL LIBRARY; CHEMICAL LIBRARY  
 Structure :



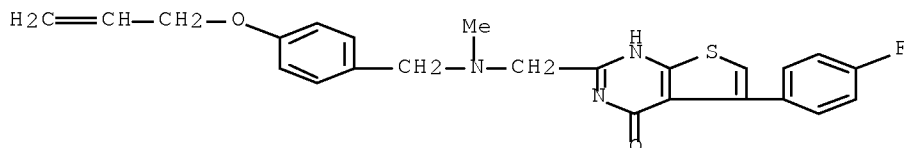
L16 ANSWER 11 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2049271778 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 13 Jun 2008  
 Order Number (ON): ken-533977  
 Chemical Name (CN): Thieno[2,3-d]pyrimidine-2-methanamine,  
 4-amino-N,5,6-trimethyl-N-[[4-(2-propen-1-  
 yloxy)phenyl]methyl]-  
 CAS Registry No. (RN): 1030752-95-4  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



L16 ANSWER 12 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048987769 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 13 Jun 2008  
 Order Number (ON): kuk-524975  
 Chemical Name (CN): Thieno[2,3-d]pyrimidin-4(1H)-one,  
 5-(4-fluorophenyl)-2-[[methyl[[4-(2-propen-1-  
 yloxy)phenyl]methyl]amino]methyl]-  
 CAS Registry No. (RN): 1013727-14-4  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



L16 ANSWER 13 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

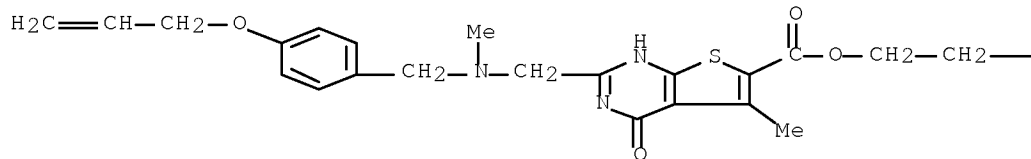
Accession No. (AN): 2048982718 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 13 Jun 2008  
 Order Number (ON): kuk-420081  
 Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,  
 1,4-dihydro-5-methyl-2-[[methyl[[4-(2-propen-1-  
 yloxy)phenyl]methyl]amino]methyl]-4-oxo-,

10/575627

2-methoxyethyl ester

CAS Registry No. (RN): 1013599-48-8  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

PAGE 1-A

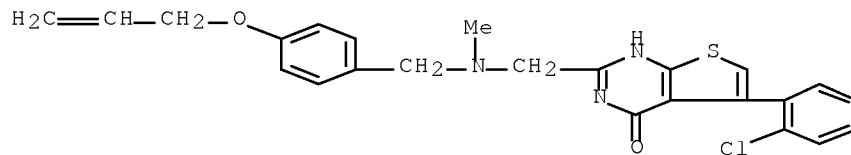


PAGE 1-B

—OMe

L16 ANSWER 14 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048968843 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 13 Jun 2008  
 Order Number (ON): kuk-420083  
 Chemical Name (CN): Thieno[2,3-d]pyrimidin-4(1H)-one,  
 5-(2-chlorophenyl)-2-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]-  
 CAS Registry No. (RN): 1013300-64-5  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

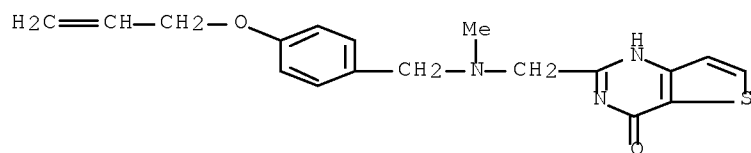


L16 ANSWER 15 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048606252 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 13 Jun 2008  
 Order Number (ON): ken-374837  
 Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,  
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 CAS Registry No. (RN): 949406-17-1  
 Supplementary Term (ST): CHEMICAL LIBRARY

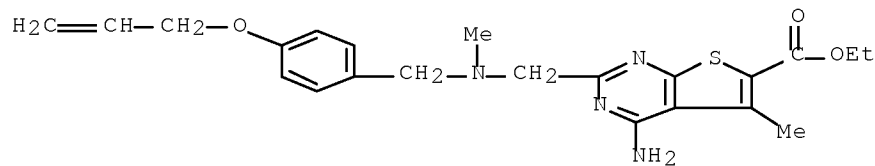
10/575627

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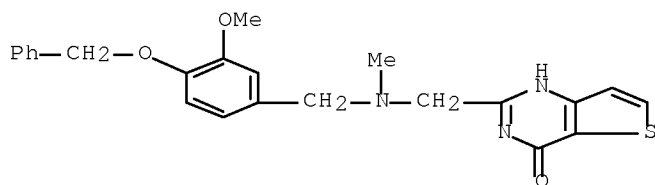
L16 ANSWER 16 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048515080 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 13 Jun 2008  
 Order Number (ON): ken-268646  
 Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,  
 4-amino-5-methyl-2-[[methyl[[4-(2-propen-1-  
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 CAS Registry No. (RN): 930905-89-8  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



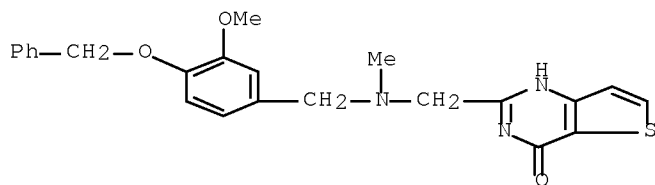
L16 ANSWER 17 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048475470 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 13 Jun 2008  
 Order Number (ON): ken-248130  
 Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,  
 2-[[[[3-methoxy-4-  
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 CAS Registry No. (RN): 930016-76-5  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



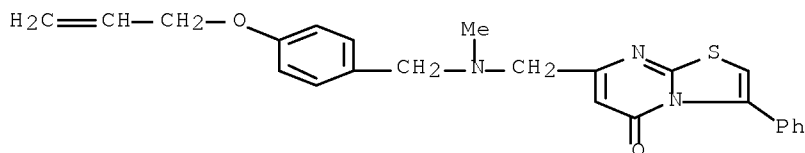
L16 ANSWER 18 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2044099010 CHEMCATS  
 Catalog Name (CO): Ryan Scientific Screening Library  
 Publication Date (PD): 25 Jan 2008  
 Order Number (ON): T5810150  
 Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,  
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 CAS Registry No. (RN): 930016-76-5  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



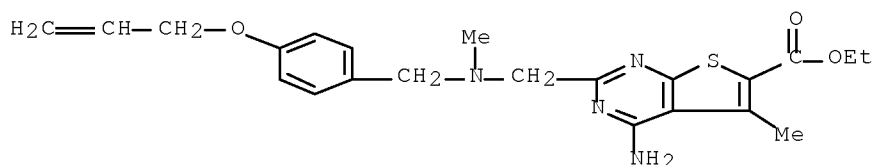
L16 ANSWER 19 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2044006130 CHEMCATS  
 Catalog Name (CO): Ryan Scientific Screening Library  
 Publication Date (PD): 25 Jan 2008  
 Order Number (ON): T5435667  
 Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
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 CAS Registry No. (RN): 871092-29-4  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



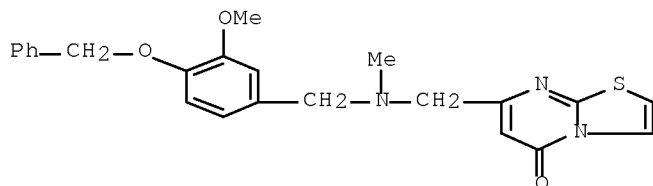
L16 ANSWER 20 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2042694057 CHEMCATS  
 Catalog Name (CO): Ryan Scientific Screening Library  
 Publication Date (PD): 25 Jan 2008  
 Order Number (ON): T5833544  
 Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,  
 4-amino-5-methyl-2-[[methyl[[4-(2-propen-1-  
 yloxy)phenyl]methyl]amino]methyl]-, ethyl ester  
 CAS Registry No. (RN): 930905-89-8  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



L16 ANSWER 21 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2042635941 CHEMCATS  
 Catalog Name (CO): Ryan Scientific Screening Library  
 Publication Date (PD): 25 Jan 2008  
 Order Number (ON): T5682113  
 Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
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 CAS Registry No. (RN): 924238-94-8  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

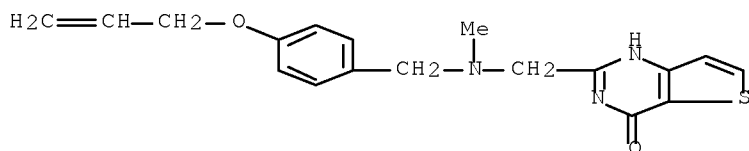


L16 ANSWER 22 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

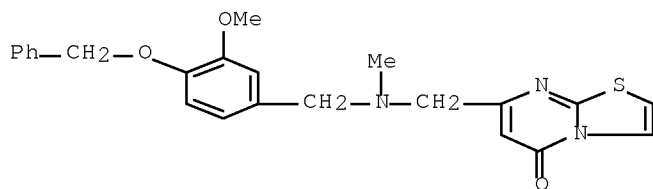
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 Publication Date (PD): 17 Jan 2008

10/575627

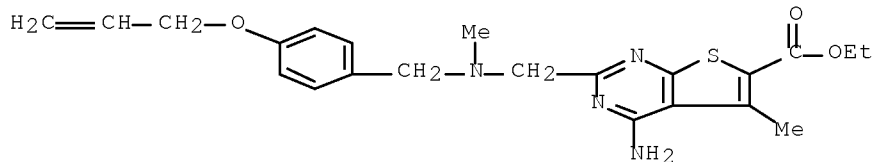
Order Number (ON): T5954092  
Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,  
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CAS Registry No. (RN): 949406-17-1  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



L16 ANSWER 23 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
Accession No. (AN): 2037934481 CHEMCATS  
Catalog Name (CO): Aurora Screening Library  
Publication Date (PD): 13 Jun 2008  
Order Number (ON): ken-092588  
Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
7-[[[3-methoxy-4-(  
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CAS Registry No. (RN): 924238-94-8  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :

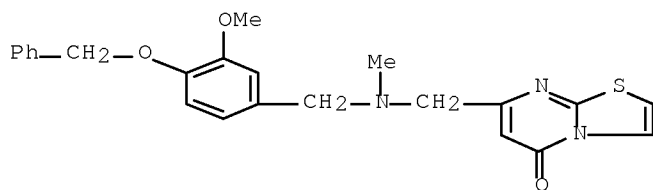


L16 ANSWER 24 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN  
Accession No. (AN): 2033762283 CHEMCATS  
Catalog Name (CO): Enamine Screening Library  
Publication Date (PD): 17 Jan 2008  
Order Number (ON): T5833544  
Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,  
4-amino-5-methyl-2-[[methyl[[4-(2-propen-1-  
yloxy)phenyl]methyl]amino]methyl]-, ethyl ester  
CAS Registry No. (RN): 930905-89-8  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



L16 ANSWER 25 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

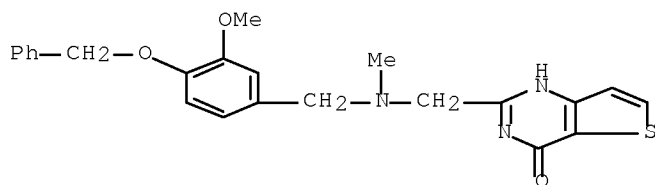
Accession No. (AN): 2033646191 CHEMCATS  
 Catalog Name (CO): Enamine Screening Library  
 Publication Date (PD): 17 Jan 2008  
 Order Number (ON): T5682113  
 Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
 7-[[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]methylamino]methyl]-  
 CAS Registry No. (RN): 924238-94-8  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



L16 ANSWER 26 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

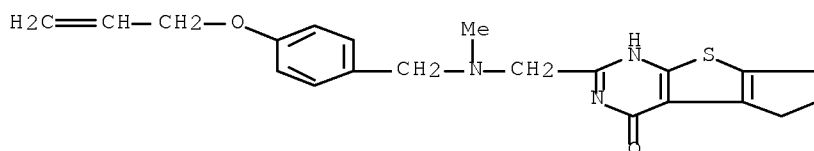
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 Publication Date (PD): 17 Jan 2008  
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 CAS Registry No. (RN): 930016-76-5  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :





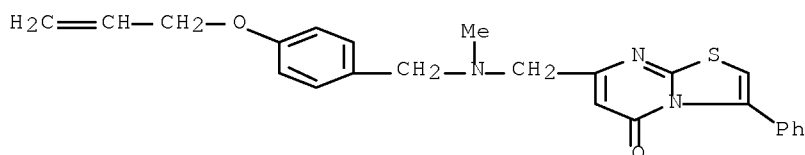
L16 ANSWER 27 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2029314936 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 13 Jun 2008  
 Order Number (ON): kend-0120483  
 Chemical Name (CN): 4H-Cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one,  
 1,5,6,7-tetrahydro-2-[[methyl[[4-(2-  
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 CAS Registry No. (RN): 876579-73-6  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



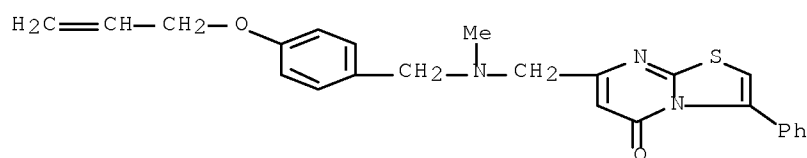
L16 ANSWER 28 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2028893097 CHEMCATS  
 Catalog Name (CO): Ambinter Stock Screening Collection  
 Publication Date (PD): 21 Nov 2008  
 Order Number (ON): T5435667  
 Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
 7-[[methyl[[4-(2-  
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 CAS Registry No. (RN): 871092-29-4  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



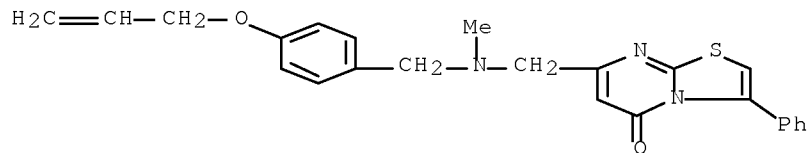
L16 ANSWER 29 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2026298900 CHEMCATS  
Catalog Name (CO): Aurora Screening Library  
Publication Date (PD): 13 Jun 2008  
Order Number (ON): kenc-0030177  
Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
7-[[methyl[[4-(2-  
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CAS Registry No. (RN): 871092-29-4  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



L16 ANSWER 30 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2025394232 CHEMCATS  
Catalog Name (CO): Enamine Screening Library  
Publication Date (PD): 17 Jan 2008  
Order Number (ON): T5435667  
Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,  
7-[[methyl[[4-(2-  
propenyloxy)phenyl]methyl]amino]methyl]-3-phenyl-  
CAS Registry No. (RN): 871092-29-4  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



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\*\*\*\*\* SEARCH HISTORY \*\*\*\*\*

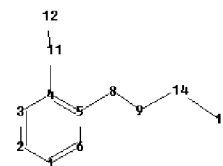
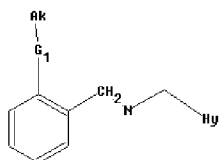
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FILE 'REGISTRY' ENTERED AT 08:13:58 ON 06 MAR 2009  
ACT DAV627MAIN/A

L1 STR

Uploading L2.str



chain nodes :  
8 9 11 12 14 15  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
4-11 5-8 8-9 9-14 11-12 14-15  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
4-11 9-14 11-12 14-15  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

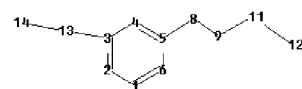
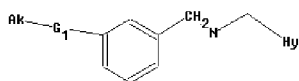
G1:O,S,N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS  
12:CLASS  
14:CLASS 15:Atom  
Generic attributes :  
15:  
Saturation : Unsaturated

Element Count :  
Node 12: Limited  
C,C1-8

L2 ( 15347)SEA SSS FUL L1  
L3 STR

Uploading L3.str



chain nodes :  
8 9 11 12 13 14  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
3-13 5-8 8-9 9-11 11-12 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
3-13 9-11 11-12 13-14  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O,S,N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS  
Generic attributes :  
12:  
Saturation : Unsaturated

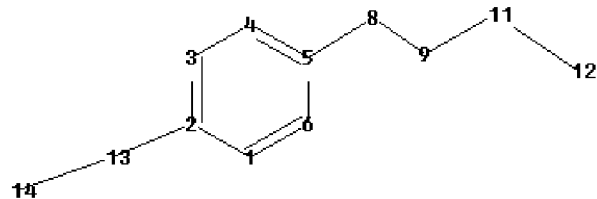
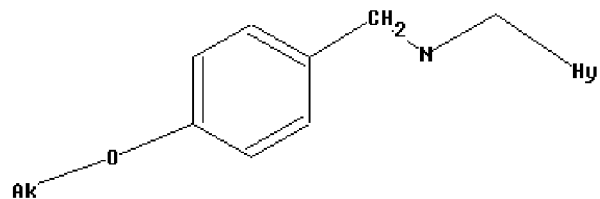
Element Count :  
Node 14: Limited  
C,C1-8

L4 ( 22405)SEA SSS FUL L3

10/575627

L5 SCR 2043 OR 1918  
L6 STR

Uploading L5.str



chain nodes :  
8 9 11 12 13 14  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
2-13 5-8 8-9 9-11 11-12 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
2-13 9-11 11-12 13-14  
exact bonds :  
5-8 8-9  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS

Generic attributes :

12:

Saturation : Unsaturated

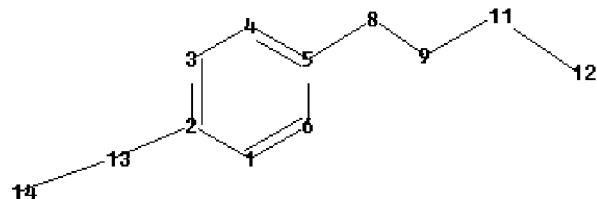
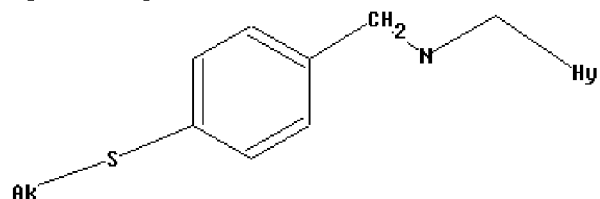
Element Count :

Node 14: Limited

C,C1-8

L7 ( 26302)SEA SSS FUL L6 NOT L5  
L8 STR

Uploading L6.str



```

chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

```

G1:O,S,N

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes :
12:
Saturation           : Unsaturated

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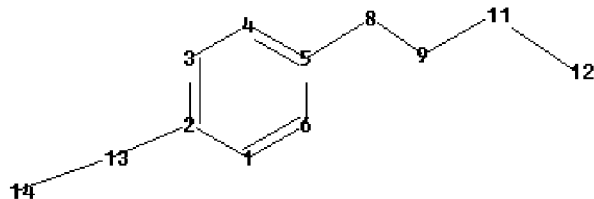
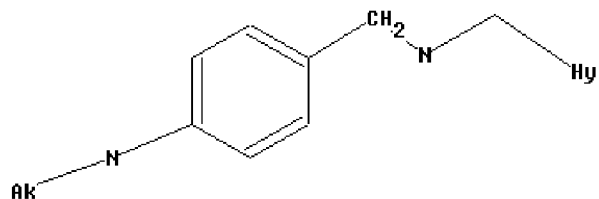
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Element Count :
Node 14: Limited
C,C1-8

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L9 STR

Uploading L7.str



```

chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14

```

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exact bonds :

5-8 8-9

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom  
13:CLASS 14:CLASS

Generic attributes :

12:

Saturation : Unsaturated

Element Count :

Node 14: Limited

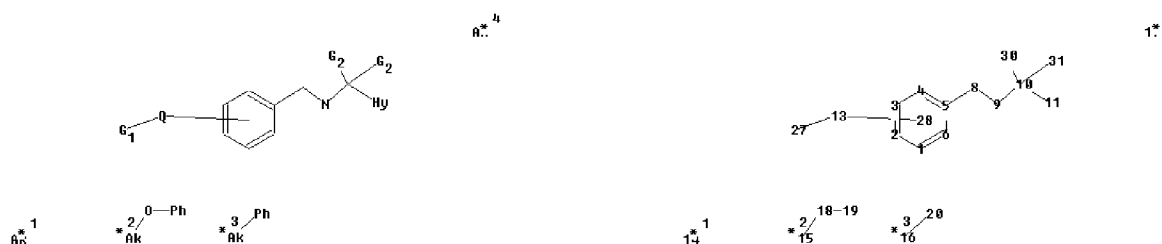
C,C1-8

L10 ( 5008)SEA SSS FUL L8 OR L9

L11 55683 SEA ABB=ON PLU=ON L2 OR L4 OR L7 OR L10

L12 STRUCTURE UPLOADED  
D

Uploading L12.str



chain nodes :

8 9 10 11 13 14 15 16 17 18 19 20 27 30 31

ring nodes :

1 2 3 4 5 6

chain bonds :

5-8 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 18-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20

exact bonds :

5-8 18-19  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6  
 isolated ring systems :  
 containing 1 :

G1:[\*1],[\*2],[\*3]

G2:H,[\*4]

Connectivity :  
 14:1 E exact RC ring/chain 17:1 E exact RC ring/chain  
 Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom  
 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
 27:CLASS 28:Atom  
 30:CLASS 31:CLASS  
 Generic attributes :  
 11:  
 Saturation : Unsaturated

Element Count :  
 Node 11: Limited  
 C,C5-10  
 S,S1

Node 14: Limited  
 C,C3-8

Node 17: Limited  
 C,C1-3

L13 1 SEA SUB=L11 SSS SAM L12  
 D SCAN  
 L14 12 SEA SUB=L11 SSS FUL L12  
 SAVE TEMP L14 DAV627REGL12/A

FILE 'HCAPLUS' ENTERED AT 08:20:42 ON 06 MAR 2009  
 L15 0 SEA ABB=ON PLU=ON L14

FILE 'CHEMCATS' ENTERED AT 08:58:39 ON 06 MAR 2009  
 L16 30 SEA ABB=ON PLU=ON L14  
 D  
 D QUE L15  
 D QUE L14

FILE 'REGISTRY' ENTERED AT 09:01:42 ON 06 MAR 2009  
 D L14 1-12 IDE

FILE 'CHEMCATS' ENTERED AT 09:01:45 ON 06 MAR 2009  
 D QUE L16

FILE 'STNGUIDE' ENTERED AT 09:02:05 ON 06 MAR 2009



10/575627

FILE 'CHEMCATS' ENTERED AT 09:02:14 ON 06 MAR 2009  
D L16 1-30 IDE

FILE 'STNGUIDE' ENTERED AT 09:02:18 ON 06 MAR 2009